

6-Mercaptopurine
50-44-2 | DTXSID0020810

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 200 °C

Global applicability domain: Inside

Local applicability domain index: 3.79e-01

Confidence level: 3.55e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pyrazine-2,3-dicarbonitrile</div> <div>Measured: 132</div> <div>Predicted: 108</div>	<div>Image not found</div> <div>Deethylatrazine</div> <div>Measured: 133</div> <div>Predicted: 143</div>	<div>Image not found</div> <div>Allopurinol</div> <div>Measured: 350</div> <div>Predicted: 287</div>
<div>Image not found</div> <div>2',3'-Dideoxyadenosine</div> <div>Measured: 185</div> <div>Predicted: 194</div>	<div>Image not found</div> <div>Brodimoprim</div> <div>Measured: 227</div> <div>Predicted: 226</div>	